Summary of WG2

Computations for Accelerator Physics

J.-L. Vay, A. Arefiev

2 plenary talks, 14 WG talks and 5 posters:

Weiming An, Alexey Arefiev, Benjamin Cowan, Alexander Debus, Brendan Godfrey, Yue Hao, Chengkun Huang, zinetula insepov, Patrick Lee, Timon Mehrling, Warren Mori, Jonathan Reyes, Brad Shadwick, Alexander Stamm, Frank Tsung (for Asher Davidson), Jean-Luc Vay, Seth Veitzer, Marija Vranic, Peicheng Yu.

Outline

PIC theory

Novel methods

Reduced PIC methods

Diagnostics in PIC

Applications

Outlook

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Review and Recent Advances in PIC Modeling of Relativistic Beams and Plasmas [Godfrey]

PIC established as credible tool for modeling advanced accelerators

AAC field is stimulating new research in PIC methodology

PIC numerical stability analyses well in hand

- Encompasses many algorithms (FDTD, PSTD, PSATD, PSAOTD, sub-cycling)
- Thoroughly validated by PIC simulations

PIC numerical instabilities can be suppressed in most instances

- Multiple approaches suppress growth rates to below $0.01/\omega_p$
- Minimal (% level) extra cost incurred

Numerical Cherenkov in boosted frame simulations

Tremendous progress since AAC 2012:

- **Analysis of Numerical Cherenkov has been generalized:**
  - **to finite-difference PIC codes ("Magical" time step explained):**
    - B. B. Godfrey and J.-L. Vay, J. Comp. Phys. 248 (2013) 33.
    - X. Xu, et. al., Comp. Phys. Comm., 184 (2013) 2503.
  - **to pseudo-spectral PIC codes:**
    - B. B. Godfrey, J. -L. Vay, I. Haber, J. Comp. Phys., 258 (2014) 689.
    - P. Yu et. al, J. Comp. Phys. 266 (2014) 124.

- **Suppression techniques were developed:**
  - **for finite-difference PIC codes:**
    - B. B. Godfrey and J.-L. Vay, J. Comp. Phys. 267 (2014) 1.
  - **for pseudo-spectral PIC codes:**
    - B. B. Godfrey, J.-L. Vay, I. Haber, IEEE Trans. Plas. Sci. 42 (2014) 1339.
    - P. Yu, et. al., arXiv:1407.0272

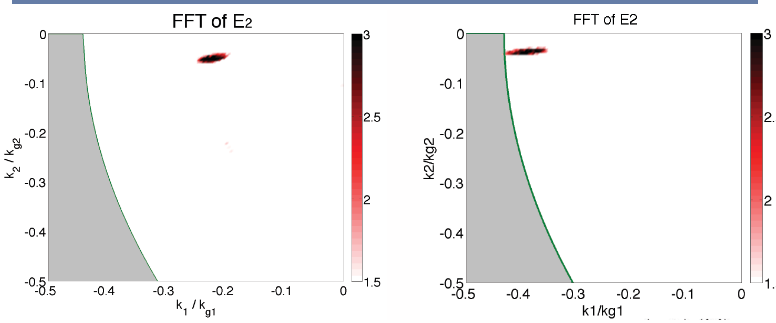
Peicheng Yu - WG2 - *Elimination of numerical Cerenkov instability for spectral EM-PIC codes*

UCLA

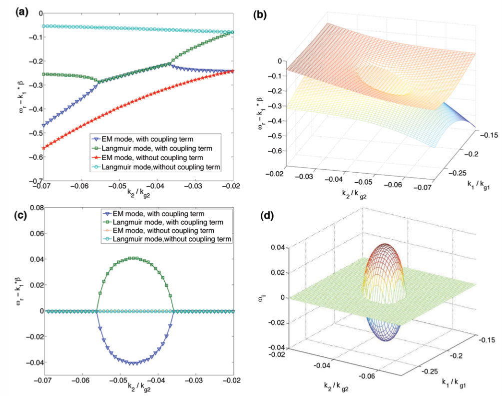
Equation for NCI

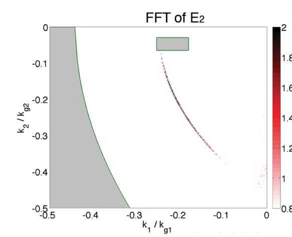
$$\left((\omega' - k_1' v_0)^2 - \frac{\omega_p^2}{\gamma^3}(-1)^\mu \frac{S_{j1} S_{E1} \omega'}{[\omega]}\right) \times$$
$$\left([\omega]^2 - [k]_{E1}[k]_{B1} - [k]_{E2}[k]_{B2} - \frac{\omega_p^2}{\gamma}(-1)^\mu \frac{S_{j2}(S_{E2}[\omega] - S_{B3}[k]_{E1} v_0)}{\omega' - k_1' v_0}\right)$$
$$+ \mathcal{C} = 0$$

eliminate (0,0) mode by reducing time or filtering

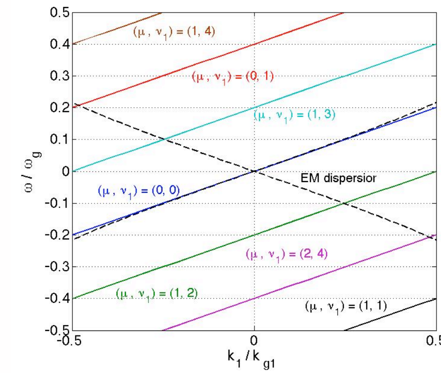


Coupling term leads to NCI

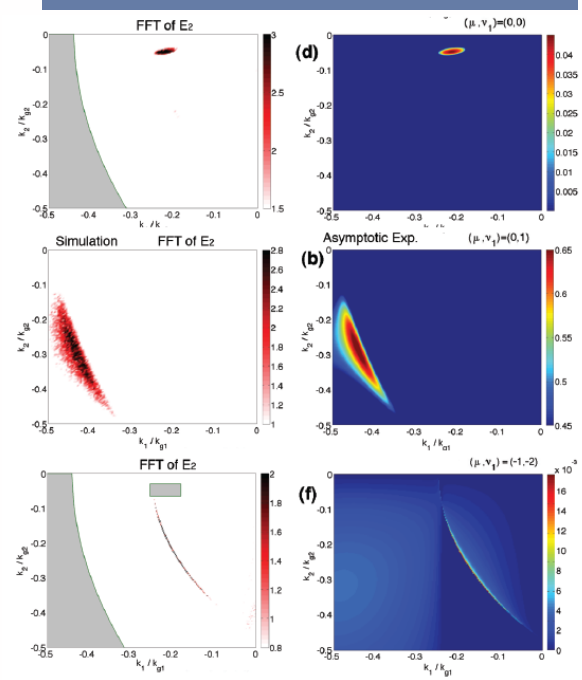




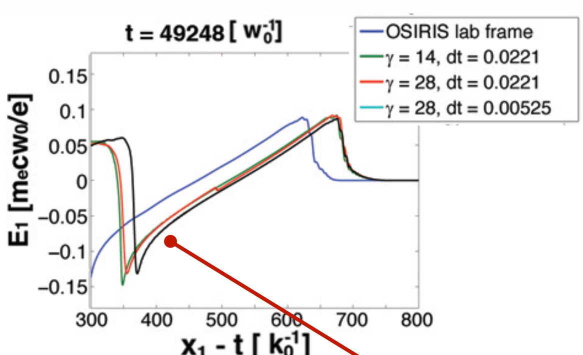
beam resonance

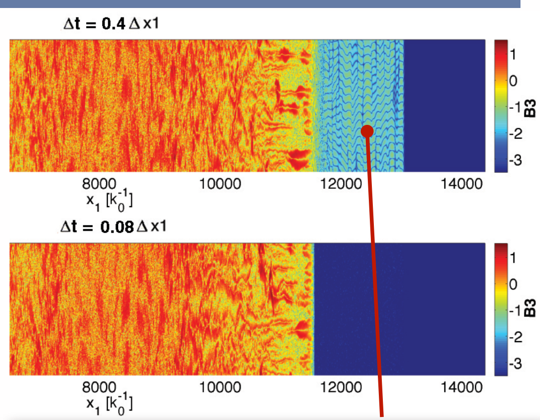


systematically study NCI modes



the strategy gives cleaner physics, and more accurate modeling





better self-injection modeling

cleaner beam

Intensity-dependent criterion for simulations of relativistic electrons in a laser field [A. Arefiev]

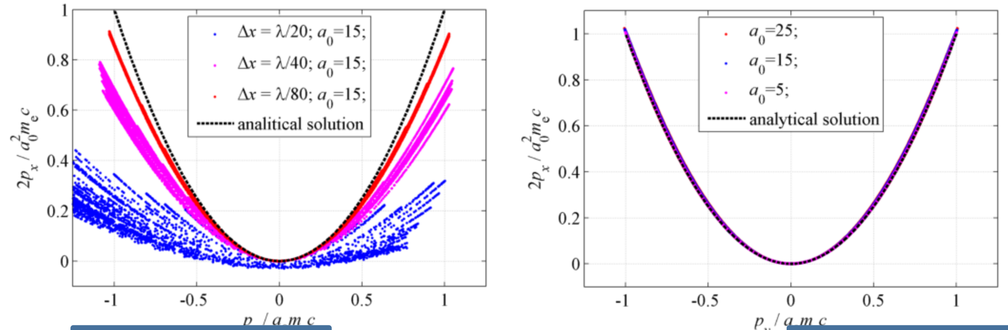
- Direct laser acceleration of electrons is important for proton acceleration, positron and neutron production etc.

- PIC electron spectra show resolution sensitivity with increased a_0.

- Strongest acceleration near stopping points causes errors in the dephasing rate and subsequent energy gain.

- The time step less than $1/\omega a_0$ is required to resolve the electron dynamics near the stopping points.

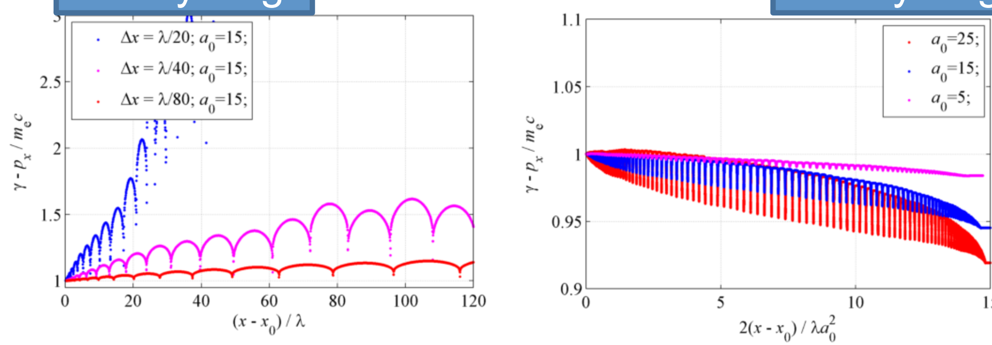
Electron momentum space



no subcycling

Electron dephasing

with subcycling



- Electron sub-cycling is a possible efficient remedy for existing PIC codes to dramatically reduce the numerical errors.

Outline

- PIC theory
- Novel methods
- Reduced PIC methods
- Diagnostics in PIC
- Applications
- Outlook

EM solver with extreme flexibility to enable runtime tuning on next generation of supercomputers [JL Vay et al]

BERKELEY LAB

Extended Warp's finite difference (FDTD) solver to arbitrary order of accuracy

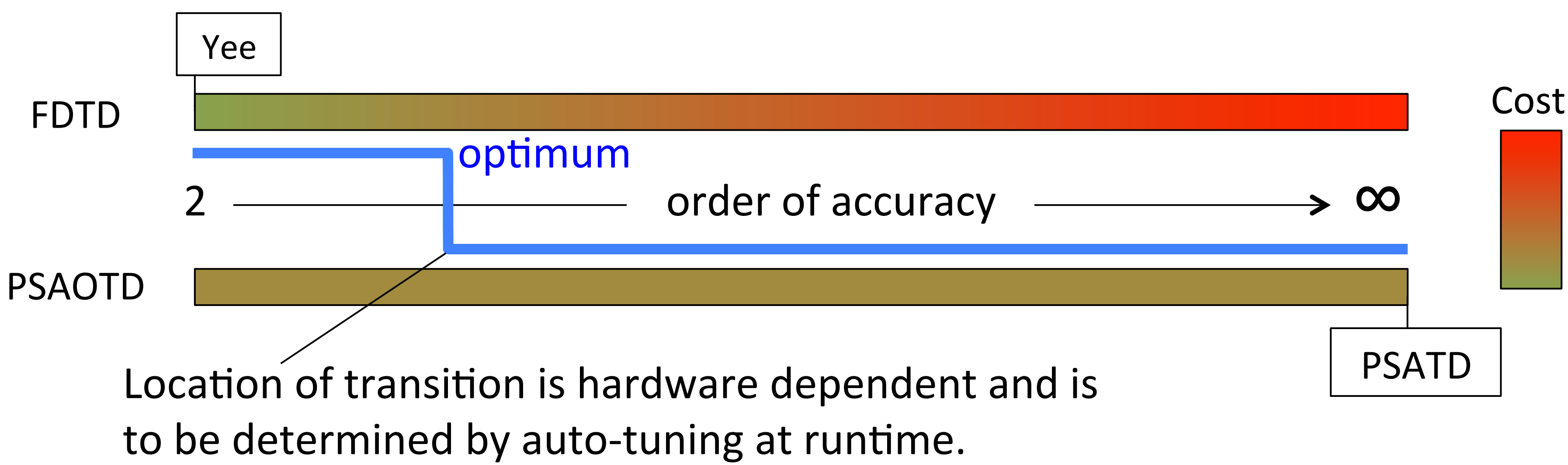
Implemented exact analytic pseudo-spectral solver (PSATD) [eq. infinite order]

Introduced new paradigm for PS solvers with local FFTs (using finite speed of light)

➔ removes difficulty of scaling global FFTs to very large number of cores

Introduced novel Pseudo-Spectral Arbitrary Order solver (PSAOTD)

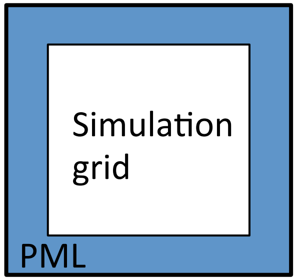
➔ unprecedented flexibility provides path to optimal solver

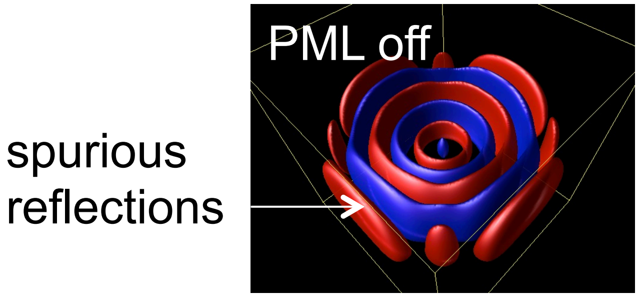


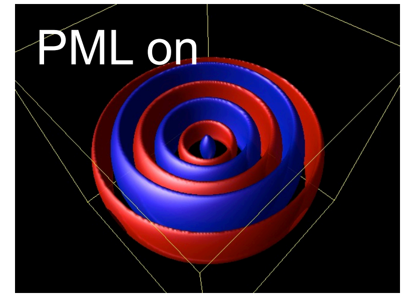
Study of Perfectly Matched Layers open boundary conditions for spectral solvers [P. Lee et al]

BERKELEY LAB

Perfectly Matched (absorbing) Layers enable the modeling of open systems

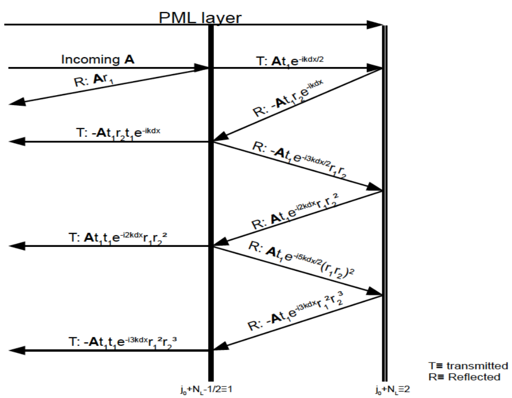


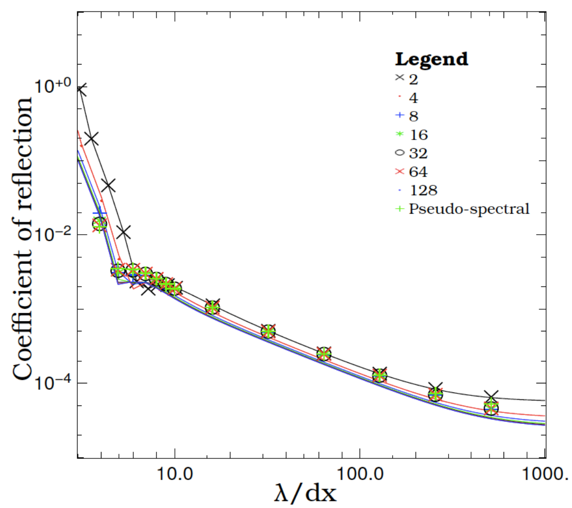


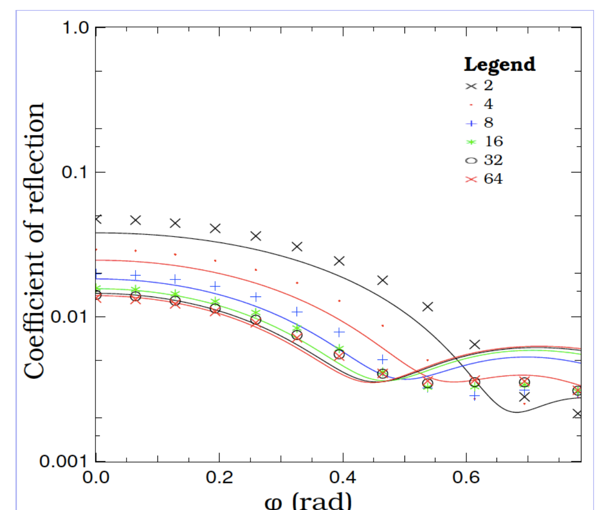


Theory was extended from order 2 to arbitrary order (spectral is limit at infinity)

Similar to Fabry-Perot







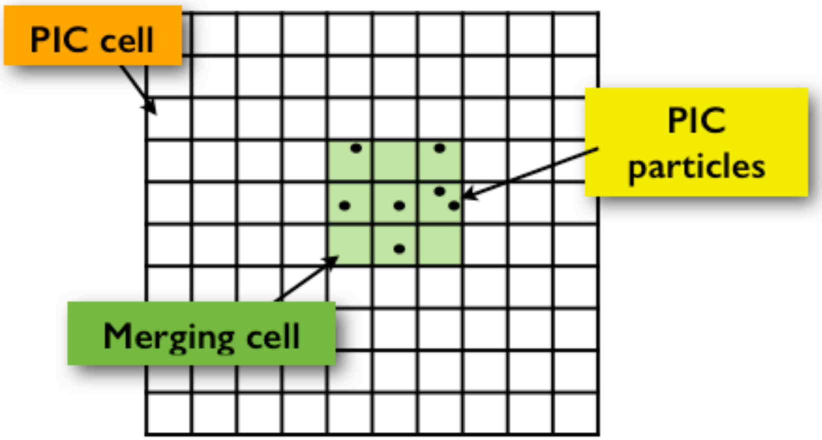
Theory consistent with numerical experiments at all wavelength & angle of incidence

Excellent absorption of PMLs at all orders and at spectral limit.

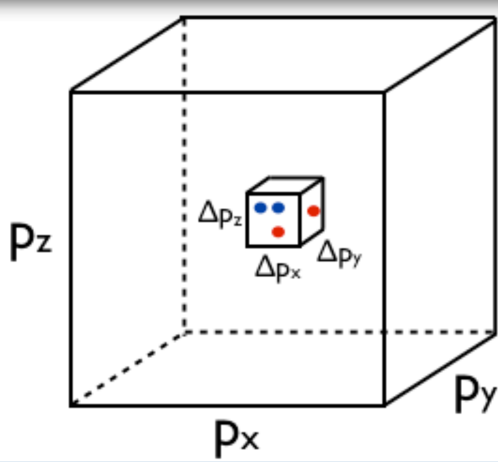
Merging algorithm for PIC - Marija Vranic

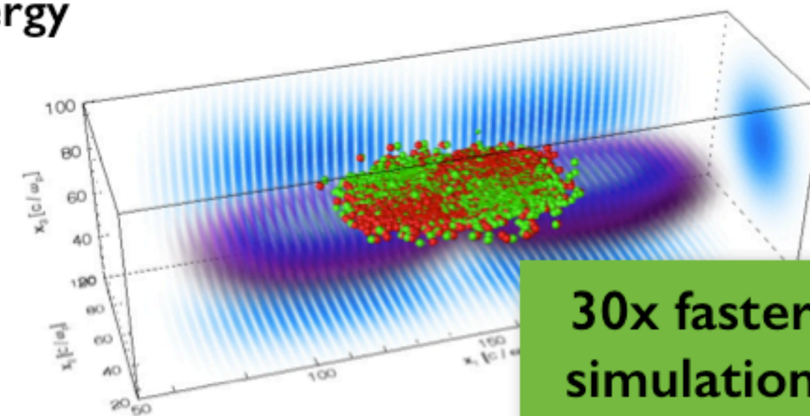
Locally conserves charge, momentum and energy

Merging particles close in 6D phasespace



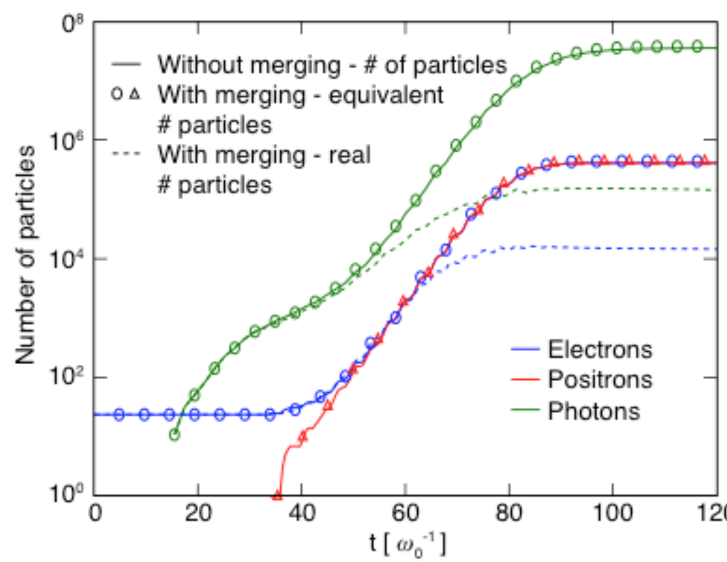
Momentum space within the merging cell





30x faster simulation

100x fewer macroparticles, same results



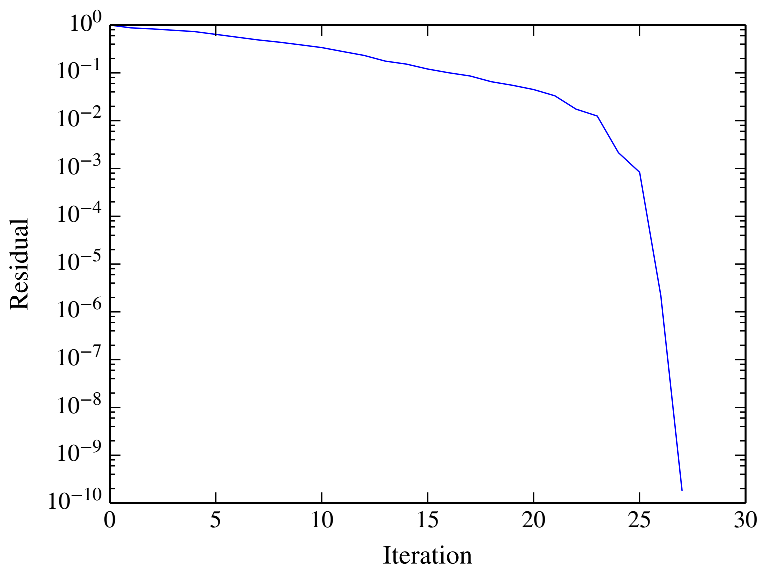
M.Vranic, T. Grismayer et al. to be submitted (2014)

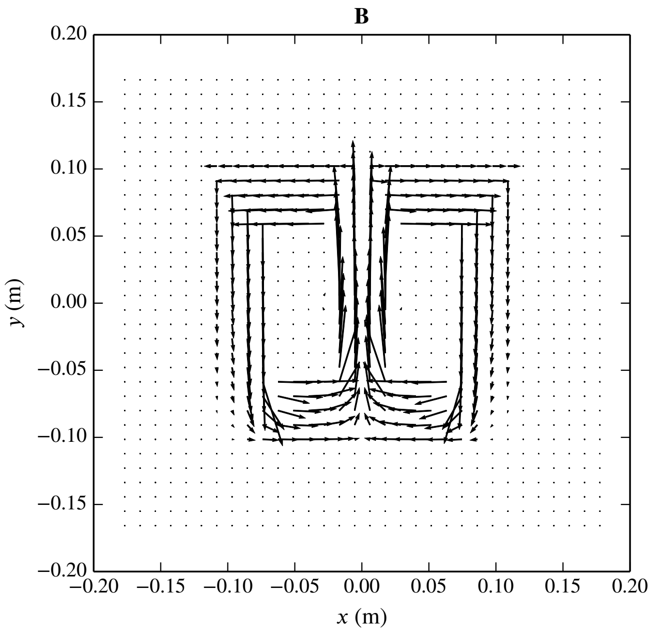
Variational Formulation of Macro-Particle Algorithms for Kinetic Plasma Simulations [Shadwick, Stamm, Reyes]

- Superset of Lewis variational formulation (70's)
- Clarified the structure of the theory by introducing a macro-particle approximation to *f* from the start:
  - ➔ allows to identify the independent choices in the theory and see how they interact,
  - ➔ path to higher spatial & temporal order is made apparent.
- Novel work on momentum conservation, charge conservation and gauge invariance
- Introduced new "true moving-window" formulation
- Formulation admits symplectic integrators on particles and fields
- Potential for energy conserving schemes
- Method developed in 1-D and examples were given

Modeling highly anisotropic, nonlinear magnetic materials [B. Cowan]

- Need to solve for magnetic field, given current
- Existing solvers fail for materials with high anisotropy and nonlinearity
- Using new mathematical techniques, we obtain convergence in 10s of iterations of an efficient iterative method





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UCLA

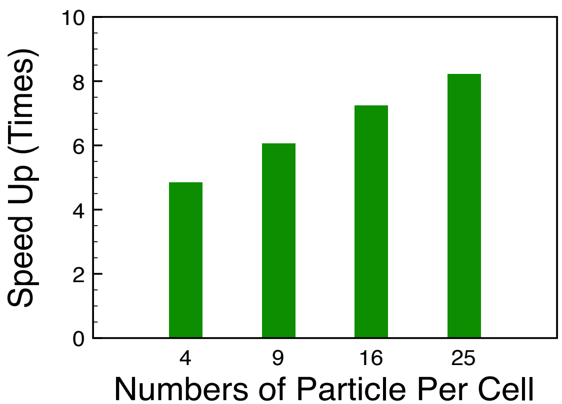
Development of QuickPIC 2.0

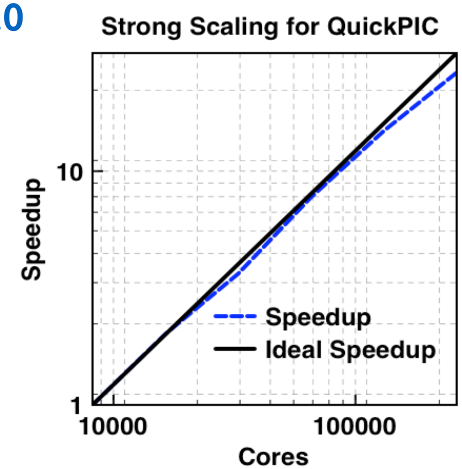
Weiming An, Viktor Decyk, Warren B. Mori (UCLA), Thomas Antonsen (UMD)

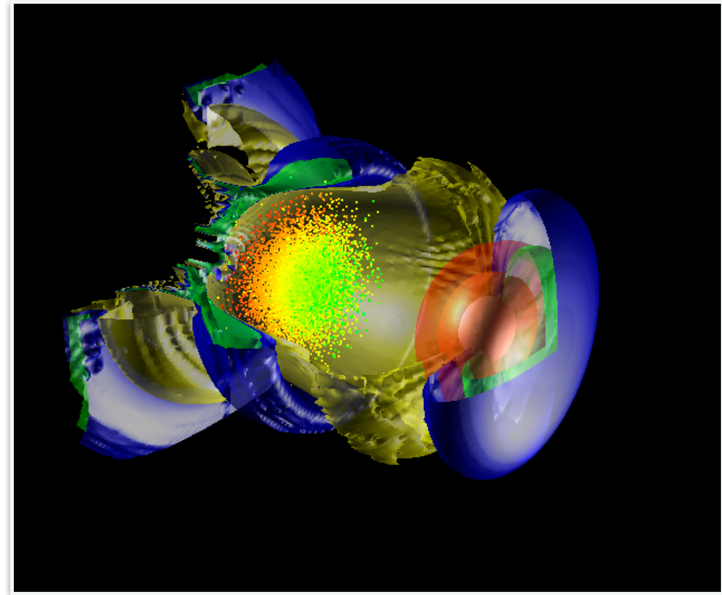
New scheme to deposit $\partial J_\perp/\partial\xi$

$$\frac{\partial}{\partial\xi}\vec{J}_\perp = \sum_i q_i \frac{\frac{\partial}{\partial\xi}\vec{p}_{i\perp}}{1-\frac{q}{m}\psi} S(\vec{x}_\perp - \vec{x}_{i\perp}) + \sum_i q_i \frac{\vec{p}_{i\perp}\frac{\partial}{\partial\xi}(\frac{q}{m}\psi)}{(1-\frac{q}{m}\psi)^2} S(\vec{x}_\perp - \vec{x}_{i\perp})$$
$$-\nabla_\perp\cdot\sum_i q_i \frac{\vec{p}_{i\perp}\vec{p}_{i\perp}}{(1-\frac{q}{m}\psi)^2} S(\vec{x}_\perp - \vec{x}_{i\perp})$$

Speedup Compared with QuickPIC 1.0



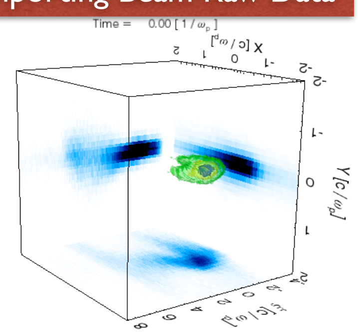




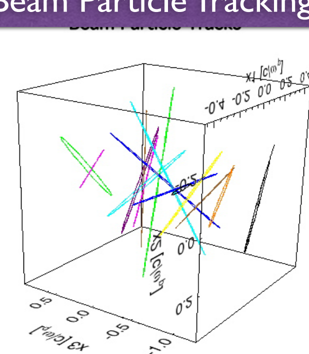
QuickPIC 2.0 simulation of LWFA with a beam load

New Initialization and Diagnostics

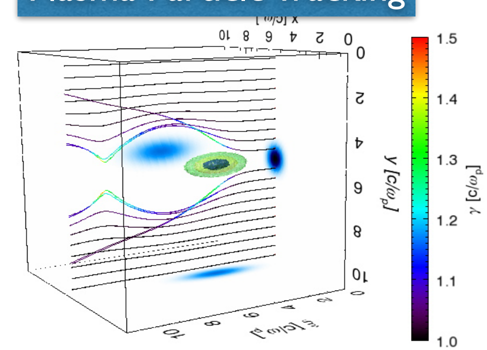
Importing Beam Raw Data



Beam Particle Tracking



Plasma Particle Tracking

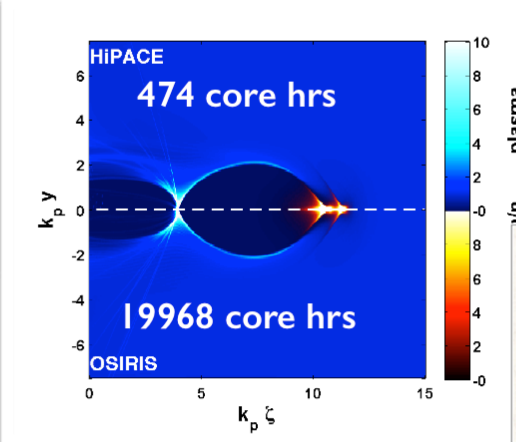


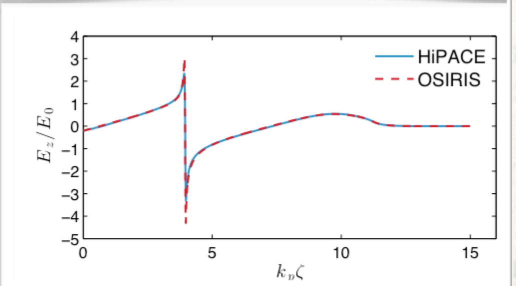
Efficient Numerical Modeling of PWFA with the Quasi-Static PIC Code HiPACE

T. Mehrling[1], C. Benedetti[2], J. Grebenyuk[1], M.J.V. Streeter[1], A. Martinez de la Ossa[1], C.B. Schroeder[2], J. Osterhoff[1]
[1] DESY, Notkestrasse 85, 22603 Hamburg, Germany [2] Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

Summary Slides

- The <u>H</u>ighly efficient <u>P</u>lasma <u>AC</u>celerator <u>E</u>mulation - HiPACE is a 3D fully parallelized, electrodynamic and relativistic quasi-static PIC code
- Dynamic time-step adjustment
- **Order-of magnitude speedup** compared to full PIC codes for adequate problems while retaining physical fidelity
- Generation of arbitrary beam phase-space distributions and import from particle tracking or full PIC codes possible





osiris v2.0

3D particle-in-cell (PIC) simulation

Advanced Accelerator Concepts Workshop 2014

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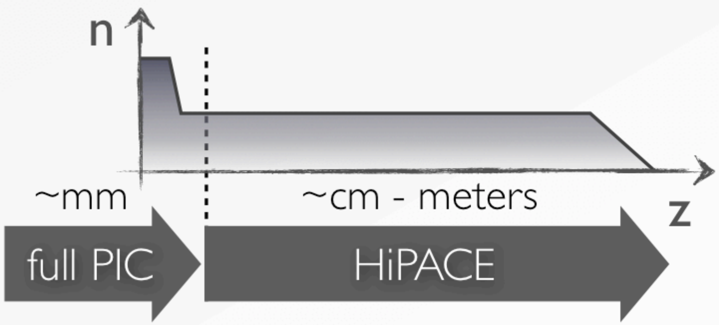
Summary Slides

- Beams can consistently be initialized **during their propagation in the plasma**
- Simulation of plasma-electron injection with a full PIC code and subsequent acceleration with HiPACE
- **Studies for FLASHForward and FACET E215 ongoing**
- **Code is currently improved in speed, functionality and stability**
  - Improvements on the (parallel) performance and parallel FFTs
  - Implementation of a laser-envelope model
  - Adding more features and functions



DESY · BERKELEY LAB · JÜLICH FORSCHUNGSZENTRUM JUQUEEN · INSTITUTO SUPERIOR TÉCNICO · Alexander von Humboldt Stiftung/Foundation · HELMHOLTZ ASSOCIATION

RZ model with azimuthal decomposition added to Osiris [F. Tsung (for A. Davidson)]

In many 3D simulations the drivers and wake develop only lower order azimuthal modes.

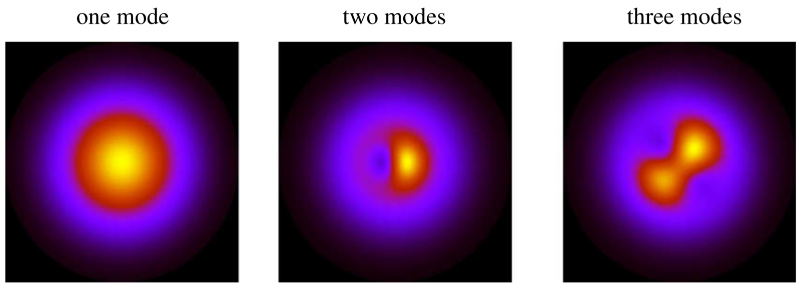
Expand in azimuthal mode number and truncate expansion! [1,2]: This is PIC in r-z and gridless in phi

Ability to expand the fields into an arbitrary number of azimuthal modes into OSIRIS.

Made improvements to [1] including rigorous charge conserving algorithm [3].

As part of OSIRIS, algorithm scales to 1,000,000+ cores and can model laser, beams, and beam loading. Allows rapid parameter scans.

[1] A.F. Lifshitz et al., JCP 228, pp.1803 (2009).
[2] B. Godfrey, M. R. C. A. NM., The IPROP Three-Dimensional Beam Propagation Code, Defense Technical Information Center, 1985.
[3] A. Davidson et al., arXiv:1403.6890



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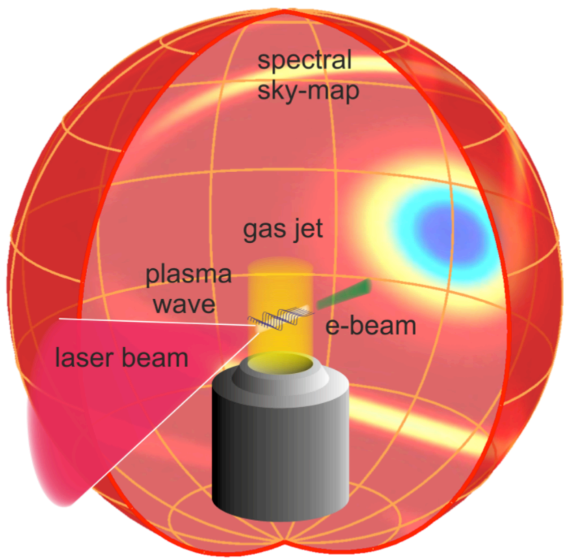
Simulating the radiation from Laser Plasma Interactions

shedding new light into the dynamics of laser-accelerated electrons

A. Debus, HZDR, Germany



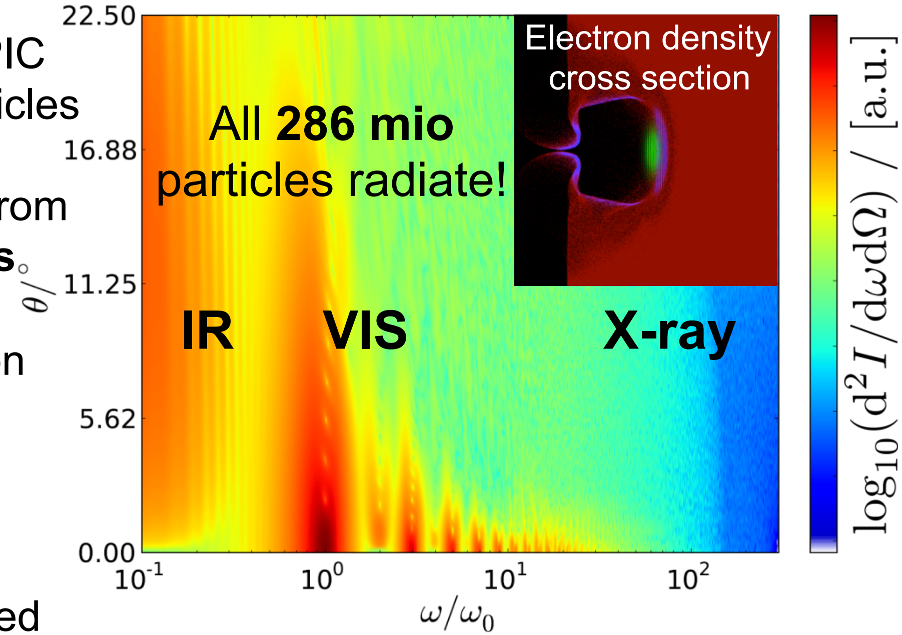
Radiation in 3D-PIC from **all** macro particles

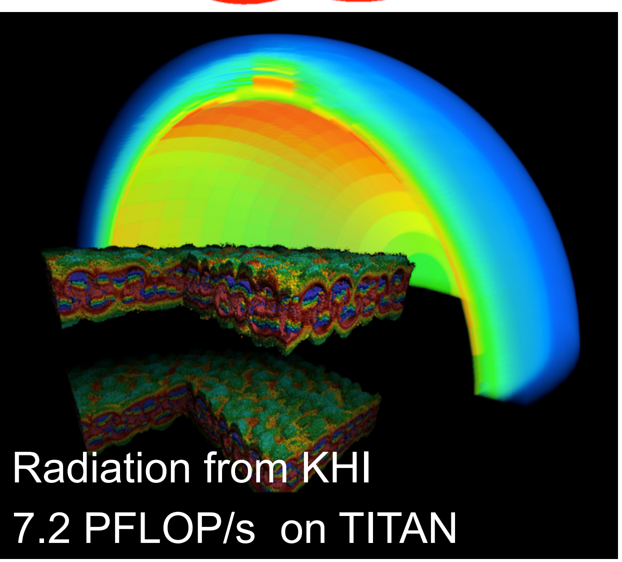
Spectrum ranges from **Far-IR to X-rays**

Many observation directions

Polarization

Full phase included



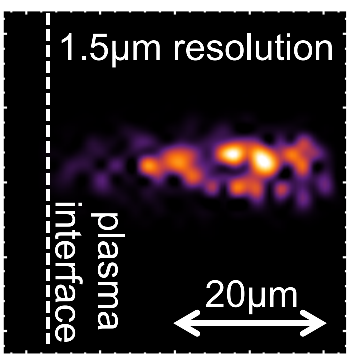


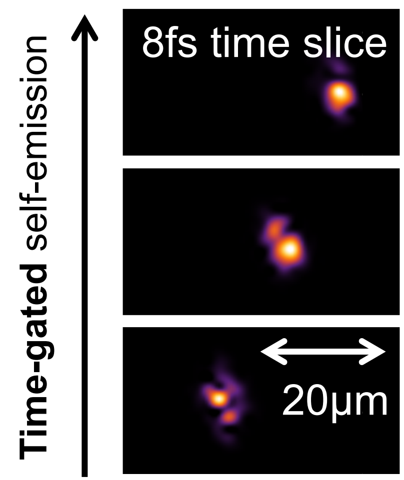
PIConGPU

A. Debus, R. Pausch,
A. Huebl, M. Bussmann
and many more…

HZDR

Time-Integrated self-emission at $2\omega_0$





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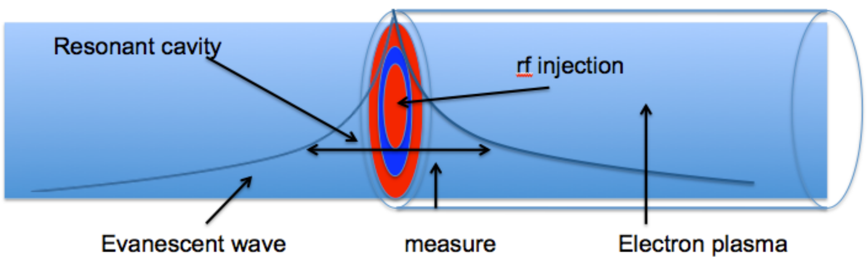
Modeling rf Resonant Cavity Method For Measuring Electron Cloud Effect Using Plasma Dielectrics

Seth A. Veitzer, David N. Smithe, Peter H. Stoltz, Tech-X Corp., Boulder, CO USA

- The resonant cavity technique will reduce uncertainties in EC measurements due to rf attenuation and reflections
- Perform detailed electrostatic PIC simulations to model plasma build-up and dissipation over one revolution period
- Derive dielectric tensor strength from electron positions
- Model rf injection *below cutoff* through time varying plasma dielectric over many thousands of revolution periods to measure sidebands



- Evanescent wave traps rf energy, providing localized sampling of electron cloud, creating a virtual resonant cavity
- The resonant frequency of this cavity depends on the EC, via the dielectric strength, which is modulated by the beam

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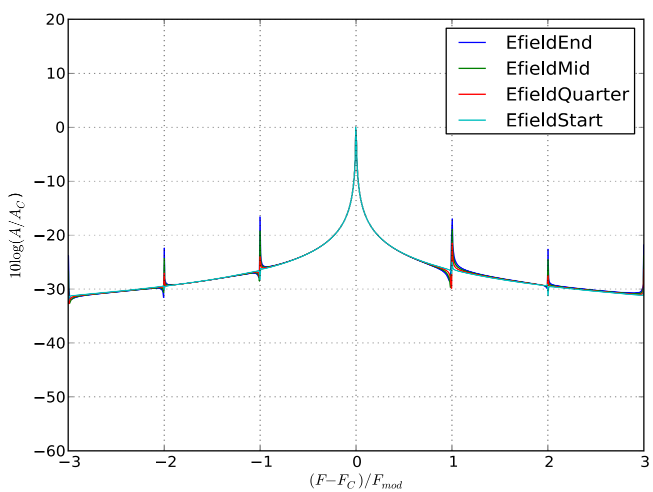
Simulated spectrum showing side bands from frequency modulation, that are generated by harmonic modulation of electron cloud density (dielectric tensor)



- First attempt to numerically model the resonant cavity technique, and compute side bands due to EC modulation
- Non-zero side band amplitude at same location as rf injection due to frequency modulation, as opposed to travelling-wave side bands, that are due to phase shifts
- Numerically stable simulations with more than 40 million time steps using dielectric models, needed to resolve 500 kHz side bands, that are otherwise not possible with kinetic PIC codes due to grid heating
- Linear increase in side band amplitudes as a function of distance from the rf source

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This work was performed under the auspices of the Department of Energy as part of the ComPASS SCiDAC-2 project (DE-FC02-07ER41499), and the SCiDAC-3 project (DE-SC0008920)

A General Model of Arcing

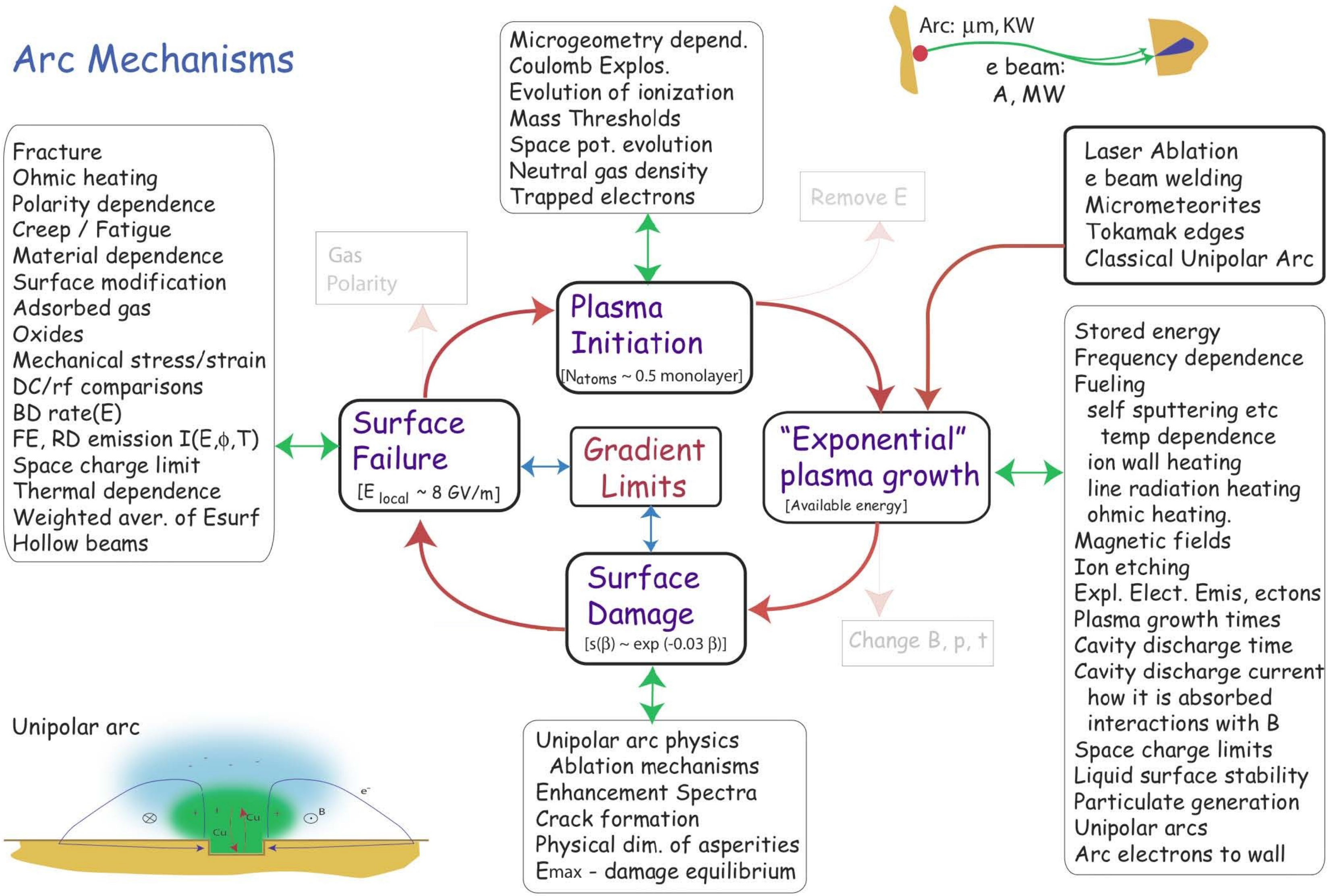
J. Norem, Z. Insepov
Nano Synergy Inc, Purdue University

Summary

- Arcing occurs in many environments, and has many common elements.
- It seems essential to understand the whole arcing process.
- It is difficult to extrapolate from narrow data sets and highly specific experiments.
- Algebraic approaches are not realistic, particularly at high densities.
- Numerical simulations can be done for all stages.
- We have published most of these results.

Summary of the Arc model

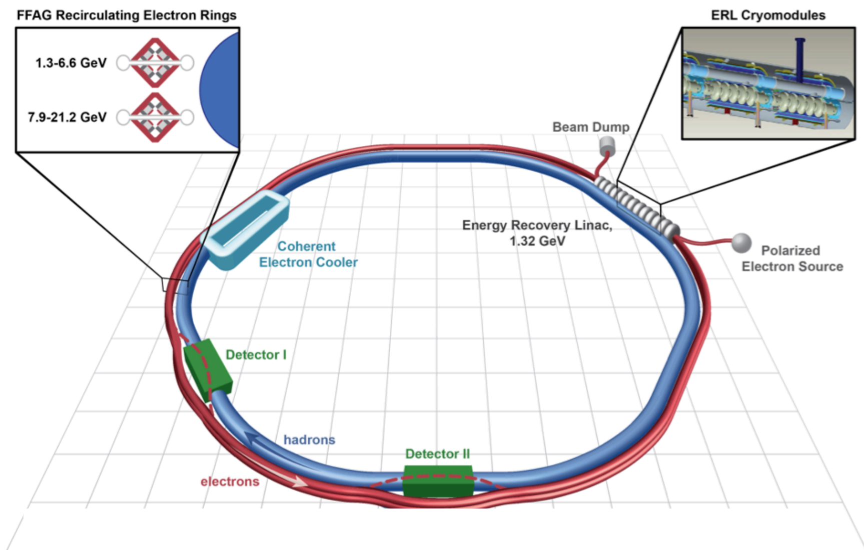
Z. Insepov, J. Norem

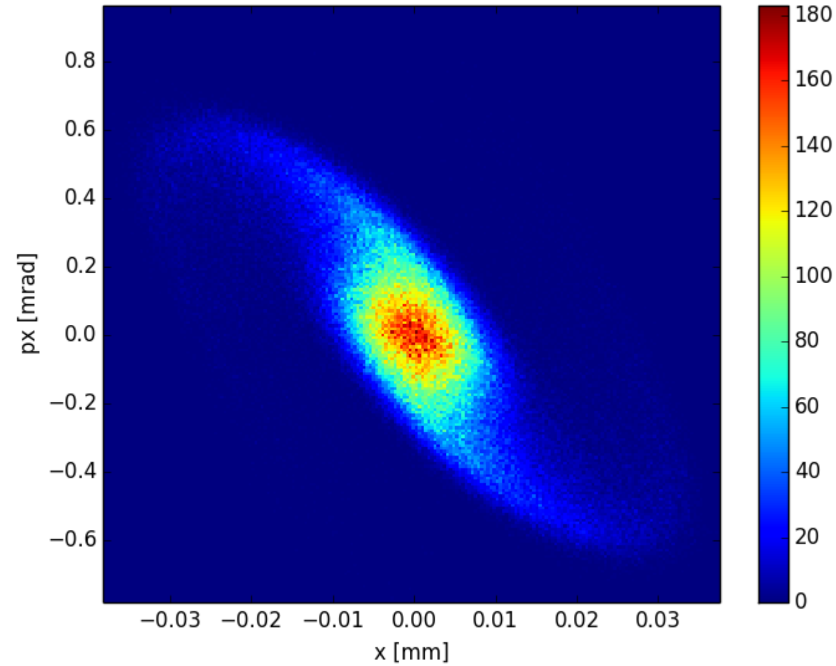


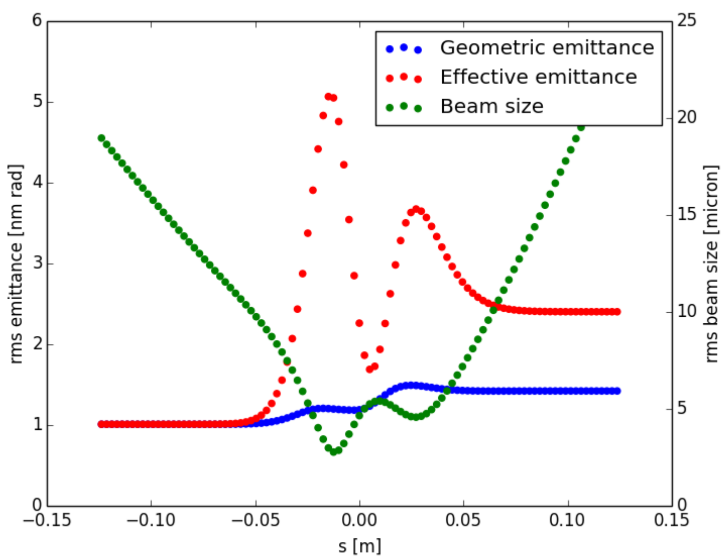
Conclusions

- Our picture of arcs is becoming simpler and more general.
- We find electrostatic fields can both trigger and drive arcs.
- Materials properties are the clue for understanding of unipolar arc formation and rf breakdown.
- We are exploring new mechanisms and news FE and atomistic models, with a number of papers underway.

Computation needs towards eRHIC
Yue Hao, BNL







eRHIC features linac-ring collision scheme that have never been proposed before

- e-beam disrupted by the ion beam
  - It is non-trivial to model the beam-beam force of the ion beam by the disrupted electron beam.
- First multi-pass ERL with FFAG energy recovery pass.

Needs / further developments

A self-consistent beam-beam/space-charge code for large-disruption beam-beam collision.

A multi-particle BBU simulation for ERL to address the effect of nonlinearity due to chromaticity and beam-beam interaction

A wrapper/interface to combine existing codes for multi-pass FFAG based ERL

Outline

PIC theory

Novel methods

Reduced PIC methods

Diagnostics in PIC

Applications

Outlook

Status, Challenges and Opportunities in Plasma-Based Acceleration Simulations [W. Mori]

Impact of simulations in AAC research not accident: result of planning, implementation, creativity and a community effort.

Many codes with many models & numerical methods: there is a community.

Mismatch between 1Hz experiments and 10^{-3}-10^{-5} Hz simulations.

➔ Can this be improved?

Tsunami (GPU, MIC, etc.) of new hardware creates challenge and opportunity:

– simulations could be reduced to seconds (or a few minutes) on 5,000 cores.

➔ real time feedback of experiments and tuning designs could be on the horizon.

Software engineering of complex code development is a grand challenge.

The challenge is to use software engineering to allow independent development of physics, high fidelity, and reduced model packages WHILE ensuring high parallel efficiency and optimization of new hardware.

➔ need community effort.

Outlook

- Simulation will continue to play a critical role in the development of AAC concepts for the foreseeable future,
- and AAC will continue to challenge and push the boundaries of simulation methods as well as codes capabilities and efficiency.
- Many codes exist and new codes continuously appear:
  - ➔ for everyone's benefit, a list of codes is being gathered for posting on web to provide live snapshot (with regular update) of simulation capabilities.
- To address its future challenges, the AAC community will need codes with more integrated physics that run fast on the next generation of computers: this demands for a more integrated effort (i.e. larger teams):
  - ➔ while there is value in diversity, duplication comes at a cost,
  - ➔ under budget constraints (e.g. P5 scenarios A&B), it may be timely to think about consolidation of efforts: common solvers, libraries, interfaces, test suites, …

Thank you

To the contributors and attendants of WG2.

To the organizers of AAC 2014.

To the funding agencies.

Let's go back to do "real work" and meet again in 2 years at AAC 2016 to report on ever better simulations methods & codes, their theory and application to the advancement of advanced accelerator concepts!